Model S506
Interactive Peak Fit

User's Manual

9230873D V1.2

ISO 9001
SYSTEM
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Interactive Peak Fit

The Interactive Peak Fit (IPF) option lets you examine the peak analysis results included in the current datasource to see whether individual peak areas are multiplet peaks, real peaks which have not been found to be statistically significant, found peaks which are not relevant to your needs, and so forth. To illustrate the capabilities of IPF, a sample CAM file, CERNIPF.CNF is included with the IPF software distribution.

IPF also lets you interactively affect the calculation of individual peak areas by editing, adding and deleting peaks and peak regions of a datasource which has been calibrated for energy and shape. If the peak analysis results are *not* included in the current datasource, IPF can act on peak regions from a datasource in the Spectroscopy Analysis application's spectral window that you select with markers.

IPF is accessible in two ways: through the Manual Menu in the Spectroscopy Analysis program and as a Batch Procedure Command.[1] IPF can be run as a peak region editor in both modes and, in the batch command mode, as a peak region viewer which can't edit the peaks.

Starting IPF

To run IPF analysis on the current datasource, select Interactive Peak Fit from the Spectroscopy Analysis application's Manual menu. This will bring up IPF's Filter Setup window (Figure 1), where you can select the Peak Filters to limit the number of peaks that IPF will display. Note that a similar dialog box allows you to change these parameters from within the IPF Peak Fitting window.

Press Execute to start IPF using the selected filters and parameters or press OK to save the parameters without running IPF.

Filters

You can use one or more of the Chi-square, FW Ratio and Multiplets filters together to limit the number of peak regions to be shown, but three of the filter selections, No Filters, Energy and Nuclide, are mutually exclusive: you can't use any other filter with them. When IPF is executed, it will present the first (lowest energy) region which matches the current filter settings.

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1. The IPFIT batch command is described in the "Batch Procedure Reference" chapter of the *Model S561 Batch Tools Support Reference Manual*.

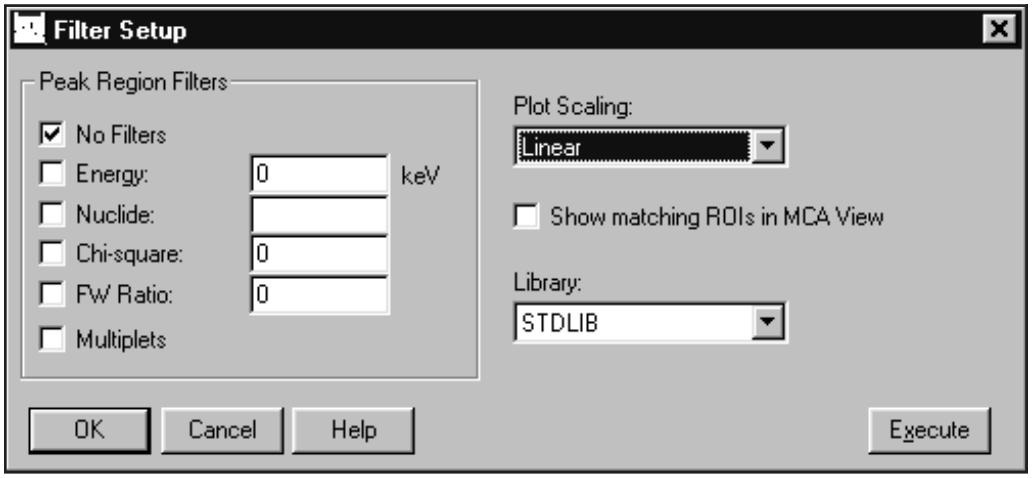

Figure 1 Filter Setup Screen

No Filters

If you choose No Filters, IPF will show all peak regions in the datasource.

Energy

If you choose the Energy filter and enter the energy of interest in its text box, IPF will show all peak regions that have at least one channel within the current datasource's energy peak match tolerance of the energy you enter here.[2] The entire region is presented as the peak region plot. If there is no peak region at that energy, a peak region equal to six FWHM, centered around the specified energy, will be established and shown as the peak region plot.

Nuclide

To look for a specific nuclide, choose the Nuclide filter and enter the nuclide's name in its text box. IPF will look in the current library for that nuclide, then will show the peak region that matches the nuclide's lowest energy. The nuclide's higher energy peaks, if any, can be seen by pressing the Next button. For each of the peaks, the entire region that includes the peak is presented as the peak region plot.

Chi-square

If you choose the Chi-square filter and enter a value in its text box, IPF will show all peak regions with a reduced Chi-square greater than that value.

2. The energy peak match tolerance is set in the Spectroscopy Analysis application, through its Calibrate | Setup dialog box.

FW Ratio

If you choose the FW Ratio filter and enter a value in its text box, IPF will show all peak regions with a measured to expected FWHM ratio greater than the given value.

Multiplets

If you choose the Multiplets filter, IPF will show only peak regions containing a multiplet.

Plot Scaling

The Plot Scaling drop-down list box lets you choose Linear, Square Root or Log scaling for the peak region (upper) plot display, as seen in Figure 2. The residuals (lower) plot, which indicates the goodness-of-fit, is always displayed as a linear plot. Both plots automatically select the appropriate vertical scale.

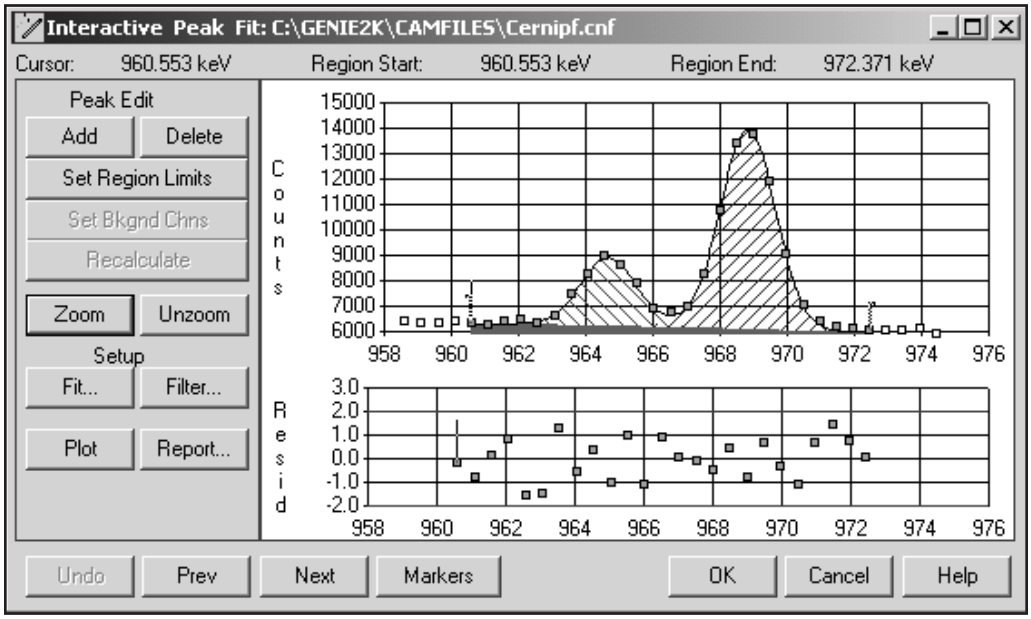

Figure 2 Peak Fitting Window

Show ROIs

If you select the “Show matching ROIs” check box and there is the Acquisition and Analysis application containing the same datasource, the ROIs that match IPF’s filter settings will be shown in the application’s spectral window when you press the Execute button. Any changes that you make to the ROIs will be seen in the spectral window according to the current filter settings after you exit IPF with an OK.

Library

The nuclide name you specified for the Nuclide filter will be searched for in the nuclide library specified here.

Using IPF

When you press the Execute button, IPF will look for peak regions in the current datasource, using the filters you selected, then display all of the peak regions it finds, starting with the region with the lowest energy.

The typical IPF window in Figure 2 shows the name of the currently selected datasource on the title bar. The window's Status Line (below the title bar) shows the location of the data cursor and the start and end of the current peak region.

Display Colors

To show specific information about the current region, IPF:

- Indicates normal channels with green squares
- Indicates continuum channels with white squares
- Shows error bars on the squares if the display scale allows
- Denotes the 2-sigma lines in the residuals display with parallel red lines.
- Differentiates peaks with a variety of colors and patterns
- Shows the continuum background as a solid magenta area
- Marks channels belonging to another region (a violated region) with blue squares
- Uses a vertical red line to mark the centroid of a deleted peak
- Uses a vertical blue line to mark the centroid of an added peak

The display includes the current peak region (upper) plot and the residuals (lower) plot, which indicates the goodness-of-fit for the displayed peak region. The data points in the residuals plot are the normalized differences between the data and the fit. A perfect fit would result in the points being displayed in a straight line with a value of zero.

If the datasource contains no peak regions that match the current filter settings, you'll see an error message telling you so; acknowledge the error message to bring up an empty plot. For IPF to show peaks, you'll have to either:

- Change the filter settings, described in "Changing the Filter Settings" on page 5.
- Or use peak regions you choose from a datasource in a Spectroscopy Analysis application's spectral window using the Markers command, described in "Markers" on page 5.

Changing the Filter Settings

To change the filter settings, press the Filter button, select different filters and exit the dialog box with an OK. Though no change will be seen in the currently displayed region, pressing either Next or Prev will make the new filter settings take effect.

Markers

Regardless of IPF's filter settings, you can select a region to view by using the markers in the Spectroscopy Analysis application's spectral window to indicate a region of interest.

When the markers have been moved to the region of interest in the spectral window, press IPF's Markers button. If the markers match the boundaries of an analysis ROI in the datasource, IPF will accept the fit of the current peak region and will change the display to the markers region as a calculated peak region with the known peak locations and fits.

If the markers do not match the boundaries of any existing analysis ROIs, the data inside the markers will automatically be selected as a new peak region, and will be displayed in the IPF window as data points. To add a peak to this region, place the IPF cursor on the peak channel, press Add, then press Recalculate to recalculate the peak area and update the peak region plot.

Previous and Next

These two controls accept the fit of the displayed peak region and move to the next lower energy (Prev button) or next higher energy (Next) peak region that satisfies the filter criteria.

Zoom and Unzoom

To look at a peak in more detail, press the Zoom button to decrease the peak region plot by five channels on each side of the peak region. To look at more of the datasource, press the Unzoom button to increase the peak region plot by five channels on each side of the peak region. Either button can be pressed several times to increase or decrease the number of channels displayed.

Peak Editing

The Peak Edit tools let you Undo an edit, Add or Delete a peak, Set Region Limits, adjust the peak fit, change the filter settings, and display a report on or generate a plot of the current region. Whenever you make any editing change, press the Recalculate button to recalculate the peak areas and to update the peak region plot.

Recalculate

Changing the region limits, or adding or deleting a peak does not affect the peak region results, so when the editing process is complete, press the Recalculate button to recalculate the peak areas and to update the peak region plot. If you try to exit IPF without refitting an edited peak, you'll see a message asking if you want to ignore the edits. Press Yes to discard the edits and exit IPF or No to remain in IPF.

Undo

If editing a peak region leads to an unacceptable result, the Undo button will discard all edits of the current peak region and will redisplay the original results of the current peak region.

Add a Peak

To add a peak to the peak region, place the data cursor at the approximate centroid channel of the new peak (in either the peak region plot or the residuals plot), then press the Add button. The added peak is shown with its centroid marked by a blue vertical bar. Press the Recalculate button to recalculate the peak area with the new peak included and update the peak region plot. Note that more than one peak may be added before recalculating the results.

Delete a Peak

To delete a peak from the peak region, place the data cursor at its approximate centroid channel, then press Delete. IPF will use the peak match energy tolerance to look for a peak location around the current location of the data cursor.

If a matching peak location is found, you'll see a message describing the peak and asking if you want to delete it. If you are satisfied that this is the correct peak, press Yes to delete it.

The deleted peak will be marked with a red vertical bar at its centroid. If this is not the peak you want to delete, press No, move the cursor to the correct peak, then press Delete again.

IPF will beep if it doesn't find a peak within the energy calibration tolerance[3] of the data cursor location. If there is more than one peak within the energy tolerance of the data cursor location, IPF will use the peak closest to the cursor.

Set Region Limits

To modify the peak region's limits, move the limit markers to new locations, then press the Set Region Limits button (the markers are moved in the same way as in the Spectroscopy Analysis application's spectral window).

Figure 3 shows a typical peak with the mouse cursor, next to the left region marker, changed to a double line with an arrow. This is the tool used to drag the marker to a new location.

When peak region limits are changed, the continuum channels will automatically be moved to be in the same locations relative to the new region limits as they were with respect to the old region limits; the number of continuum channels will remain unchanged.

If the modification of the peak region limits now includes a peak or peaks that originally were part of an adjacent peak region they will become part of the new region. If an adjacent peak that has now become part of the current peak region was originally a singlet, its original results will be erased when you press the Recalculate button.

If the adjacent peak that has been moved to the current peak region was originally part of a multiplet, its original results will be erased when you press the Recalculate button. However, the results for other peaks in the multiplet that were not moved to the current peak region will remain unchanged. The original peak region limits of the adjacent region will remain the same (even if they overlap the current peak region). If all peaks in an adjacent peak region are moved into the current one, all of its original results (including peak region limits) will be erased when you press the Recalculate button.

3. The energy calibration tolerance is set in the Spectroscopy Analysis application, through the Calibrate | Setup dialog box.

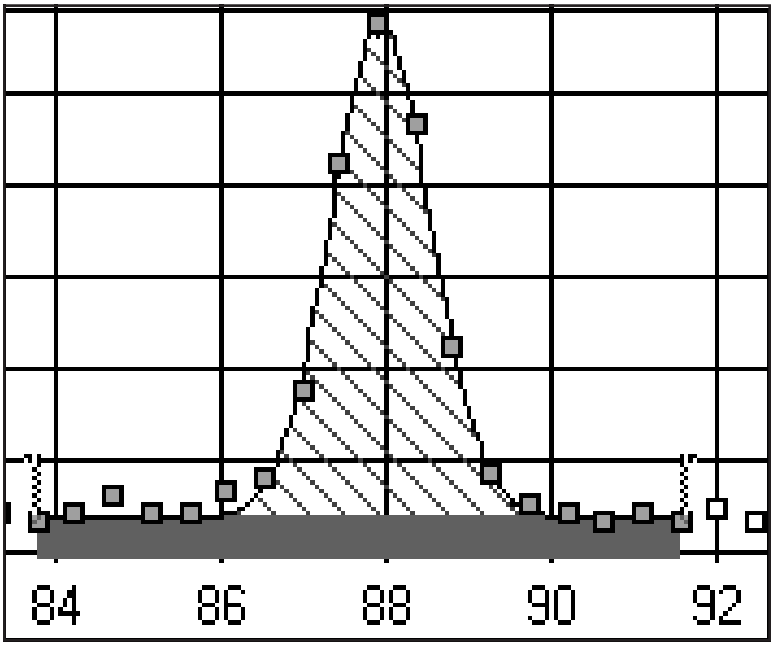

Figure 3 A Typical Peak With Region Markers

If the adjacent peak region satisfies the filter criteria and would be looked at next (after the results of the current peak region have been accepted), the following rules apply:

1. If the adjacent peak region was originally a singlet, and its only peak was moved into the current peak region, or was a multiplet and all of its peaks were moved to the current peak region, IPF will move on to the next available peak region that satisfies the filter criteria.

2. If the adjacent peak region was originally a multiplet, only some of its peaks are moved to the current peak region, and the remaining peaks in the adjacent region satisfy the filter criteria, the adjacent peak region will be presented as the next region if you move in that direction with the Next or Prev buttons.

3. Extending either of the current region's limits so that it overlaps, but does not completely include, another region creates a "violated" region.

Pressing the Next (or Previous) button when a violated region is being displayed brings up an error message telling you that a violated region exists. Answering No to the message leaves the violated region on display; answering Yes will display the next (or previous) region.

If you try to exit IPF with an OK before you have corrected the violations, you'll see a message telling you that you can't save this datasource because of the violated regions. You'll have to either go to each violated region (Yes) to correct the violation or exit without saving the changes (No).

Fit

Press the Fit button to use the current Peak Fit algorithm to adjust the fit settings for the current peak region. After making a change in the fit settings, press the Recalculate button to recalculate the current region's peak areas and to update the peak region plot.

Sum/Non-Linear LSQ Peak Fit

The Sum/non-linear LSQ Peak Fit algorithm setup, shown in Figure 4, lets you select a different peak fit algorithm, change the method of calculating the current region's continuum, and select the number of continuum channels to be used in the fit calculation.

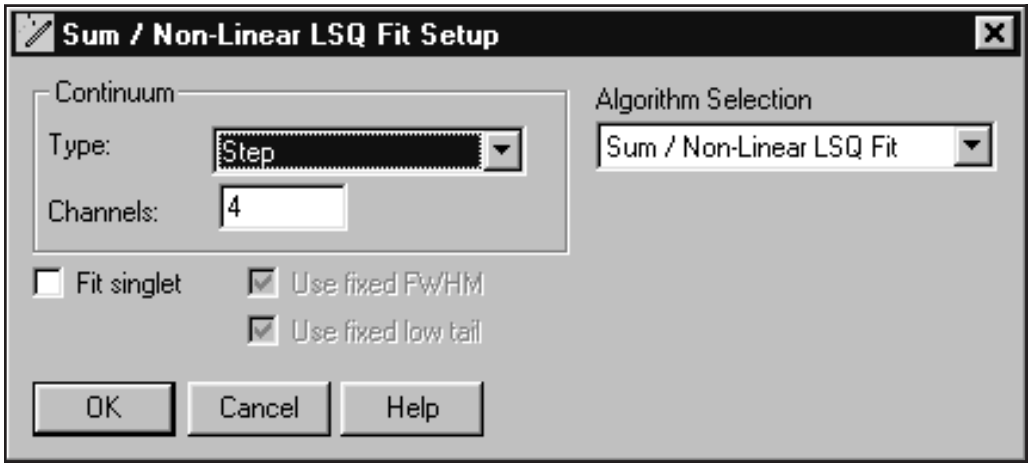

Figure 4 The Sum/Non-Linear LSQ Peak Fit Setup

The Area Non Linear LSQ Peak Fit algorithm calculates the peak areas of single peaks using the summation method described in "Peak Area for Single Peaks" in the "Algorithms" chapter of the *Genie™ 2000 Customization Tools Manual*, and the peak areas of multiplets using a fitting method, as described in "Peak Area for Multiplets" in the same document.

Algorithm Selection

The Algorithm Selection drop-down list box lets you select a different Peak Fit algorithm.

Continuum Type

You can calculate the continuum under the peaks in one of two ways: with a Step function or a Linear function. The Linear function estimates the continuum under the peaks as a trapezoid and is a simple, straightforward equation that is adequate when the continuum in the spectrum is relatively flat. The Step function should be chosen if there are any regions in the spectrum where the continuum is significantly higher on the left hand side of a peak region than on the right hand side. This function automatically reduces to a flat line if the continuum is flat.

Continuum Channels

The Channels text box lets you select the number of continuum channels on either side of the current peak region. If you have two peaks that are close together, reducing the number of continuum channels may give better results.

If you have poor peak statistics and there are no other peaks nearby, increasing the number of continuum channels establishes the continuum more accurately but makes it more likely that close lying peaks will be considered as a multiplet instead of as a singlet.

Fit Singlet

Typically, the Sum/non-linear LSQ Peak Fit routine is set up to fit multiplet peaks, but if you check the Fit Singlet check box, singlets will also be fitted, rather than calculated using the summation method.

Fixed Parameters

Selecting the Fixed FWHM Parameter or Fixed Tail Parameter check box causes the expected value (FWHM or Tail, or both) to be used for all multiplet peaks instead of allowing the value to vary for best fit. If either or both of these check boxes is not checked, the specified parameter will be allowed to vary.

Library (Gamma-M) Peak Fit

The Gamma-M Library Peak Fit algorithm, shown in Figure 5, includes steps for defining the background continuum using the erosion technique, as well as calculating the peak areas and their uncertainties.

Algorithm Selection

The Algorithm Selection drop-down list box lets you select a different Peak Fit algorithm.

Peak Search Region

You can limit the region by entering specific channel numbers in the Start and Stop text boxes.

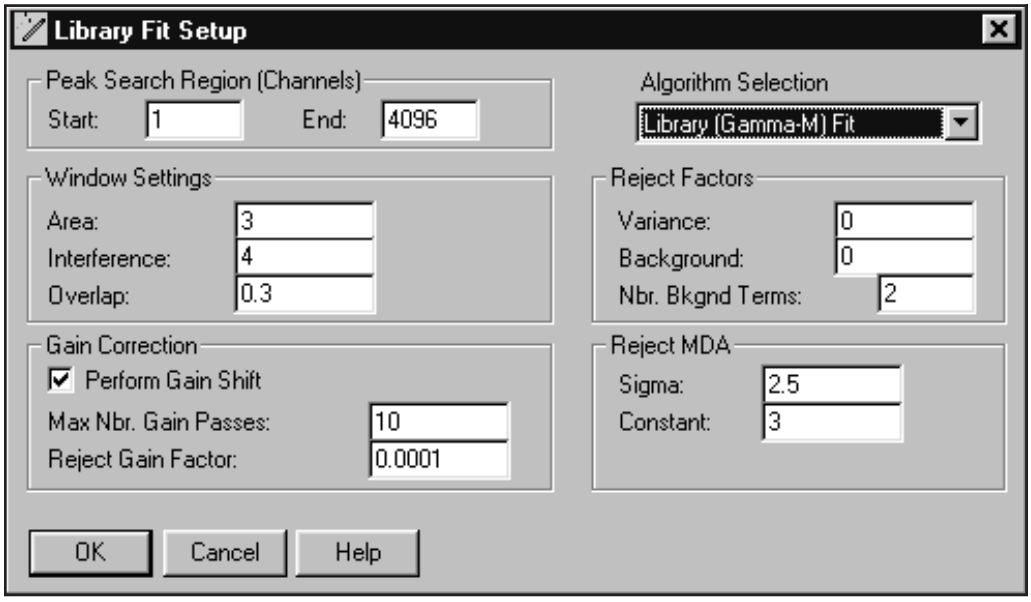

Figure 5 The Library Peak Fit Setup

Window Settings

The Area parameter specifies the FWHM multiplier used to establish the left and right ROI limits around the peaks which determine whether the peak is present in the spectrum.

The Interference parameter specifies the FWHM multiplier to establish the limit beyond which two adjacent peaks are no longer considered to interfere with each other.

The Overlap parameter specifies the FWHM multiplier which establishes the limit below which two adjacent peaks are considered to be so close that no interference correction for area overlap is calculated.

Gain Correction

The Perform Gain Shift parameter check box must be checked for these two parameters to be used in the calculations.

The Max. Nbr. Gain Passes parameter specifies the maximum number of iterations allowed for the fits.

The Reject Gain Factor parameter specifies the convergence criterion. When consecutive iterations produce a change in the Chi-square less than this value, a convergence has been achieved.

Reject Factors

The Variance parameter specifies the peak height variance rejection factor. Only peaks whose height is larger than this factor times the uncertainty of the height (at 1 sigma) will be accepted as valid peaks.

The Background parameter specifies the peak rejection factor based on the height of the background. Only peaks whose square of the height is larger than this factor times the height of the background will be accepted as valid peaks.

The Nbr. Bkgnd Terms parameter defines whether the fits are to be made with an added constant or linear continuum. 0 means that no additional continuum term will be used, 1 means that only a constant continuum will be used, and 2 means that a linear continuum will be used.

Reject MDA

The Sigma parameter specifies the multiplier of the MDA equation to accept or reject a library peak in the spectrum.

The Constant parameter specifies the constant term of the MDA equation to accept or reject a library peak in the spectrum.

Filter

If you find that more peaks are being displayed than you want to consider, you can change the peak filters from within IPF by pressing the Filter button. You'll see a dialog box similar to the one in Figure 1, which is described in "Starting IPF" on page 1. The only difference is that you'll close the dialog box with an OK instead of an Execute. To apply the new filter settings, press Prev or Next.

Report

Pressing the Report button brings up the Fit Region Report shown in Figure 6, which displays more information about the current peak region. The report window can be moved if it is covering a part of the IPF window that you'd like to look at.

Note that the items labeled "Iterations" and "Chi-square" will be zero for all single peaks that are analyzed for areas with a summation method.

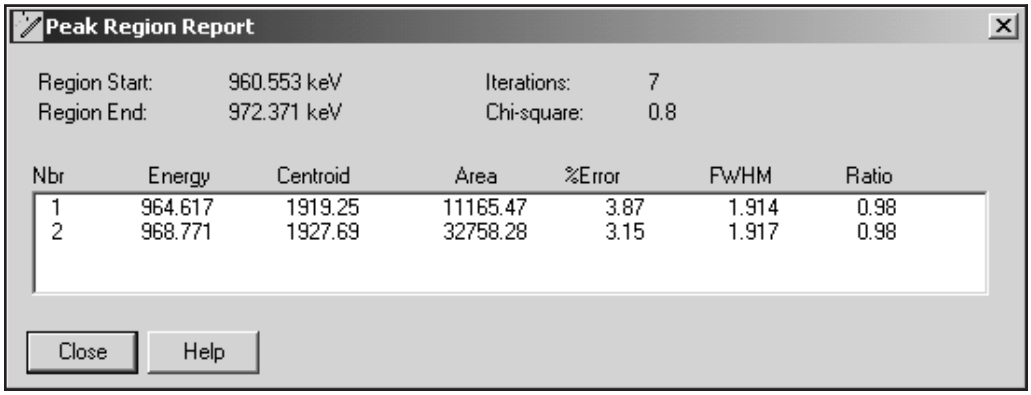

Figure 6 A Typical IPF Report

Plot

Press the Plot button to output a plot of the current peak, its residuals, and a header. Figure 7 on page 14 shows the information included in a typical plot.

Set Bkgnd Chns

The Set Background Channels function is enabled only if the current peak fit algorithm supports independent left and right background channels.

To set new background channels, position the left and right markers on one side of the region so that they enclose the new continuum channels on that side, then click on Set Bkgnd Chns. Repeat this process on the other side of the region if you want to set new background channels there as well.

Note that there can be no overlap between the continuum channels and the peak region itself, but there can be a gap between the continuum channels and the peak region.

Batch Procedure Command

In addition to using IPF in the interactive mode, you can run it with a Batch Procedure Command. For more information on batch procedures, refer to the “Batch Procedure Reference” chapter of the *Model S561 Batch Tools Support Reference Manual* with specific reference to the IPFIT command and its qualifiers.

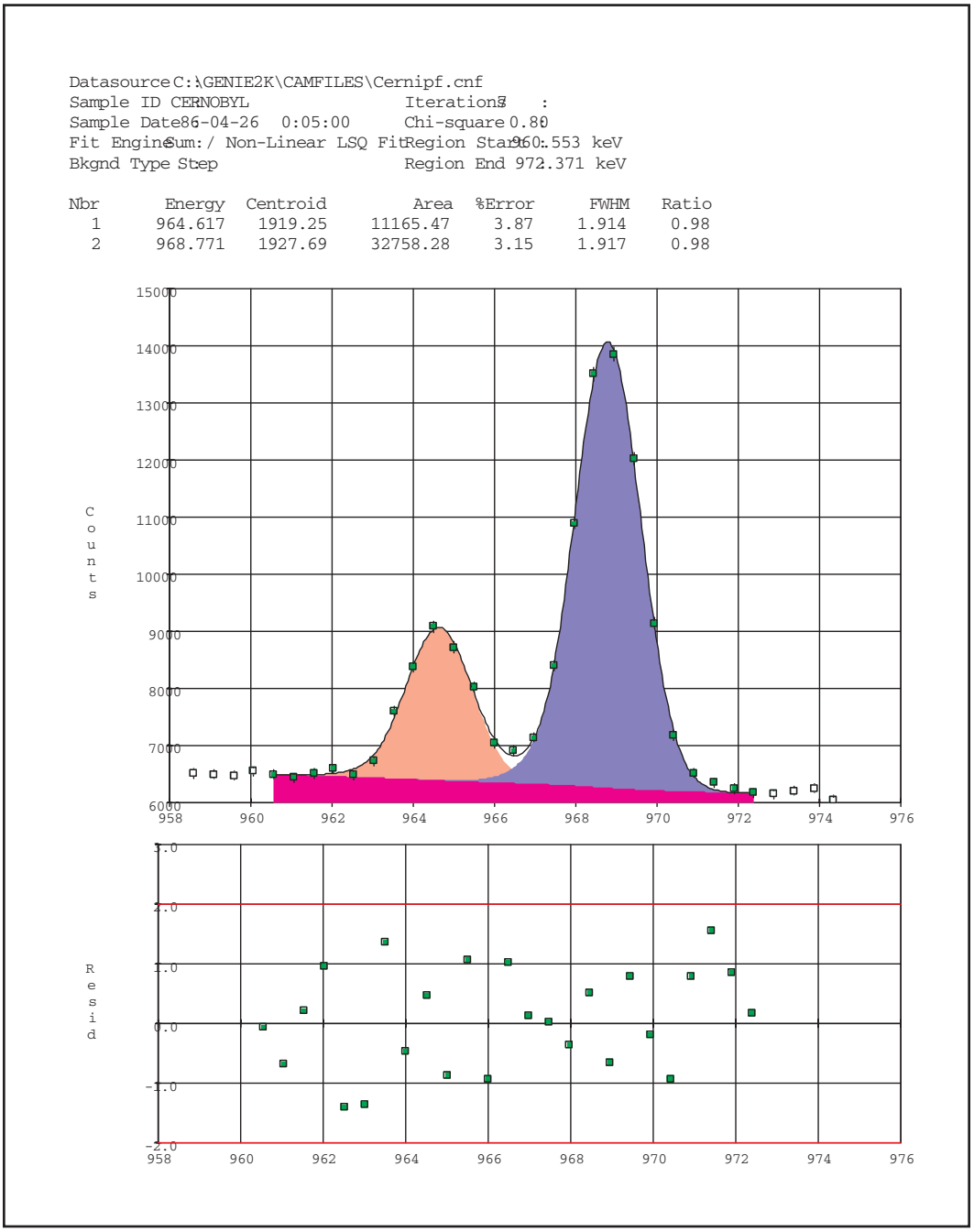

Figure 7 A Typical IPF Plot

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